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Wavelet and Isotonic Regression

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Abstract

Consider the model:

$$y_i = f(t_i) + z_i$$

where f is a decreasing function and $\{z_i\}$ are assumed to be a stationary Gaussian process with mean zero and variance σ^2 . We propose a simple thresholding procedure based on the fact that the wavelet coefficients for f , under Haar basis, are non-negative. We show that our estimator is competitive with the Grenander estimator both theoretically and numerically (in the sense of mean-square-error).

Key Words and Phrases: Isotonic Regression; Monotone Curve; Grenander Estimator; Orthogonal Wavelet Transformation; Shrinkage Estimator.

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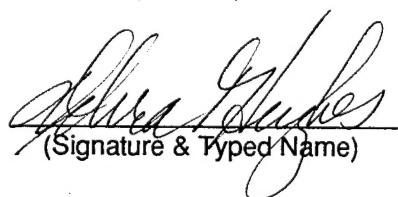
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1 Introduction

Consider the non-parametric regression model:

$$X_i = f(t_i) + z_i \quad i = 1, \dots, n \quad (1)$$

where f is only known to be a decreasing function, $t_i = i/n$ and $\{z_i\}$ are assumed to be a stationary Gaussian process with mean zero and variance σ^2 . This kind of regression problem is referred as *isotonic* regression. Examples and interpretations of such models can be found in Barlow *et al* (1972).

Let $f_i = f(t_i)$ and $f = (f_1, \dots, f_n)'$ be the sampled version of f . For simplicity we assume that $n = 2^m$ is dyadic. Our goal is to find an estimate \hat{f} depending only on X_1, \dots, X_n with small mean-squared-error:

$$R(\hat{f}, f) \equiv n^{-1} \sum_{i=1}^n E(\hat{f}_i - f_i)^2$$

In this paper, we will discuss the following 3-step wavelet shrinkage procedure, introduced by Donoho and Johnstone (1992a, b), for estimation of f :

[1] Take the Haar (the simplest wavelet) transform of X_i 's to get the empirical wavelet coefficients, $\{y_{j,k}\}_{j=0, \dots, m-1, k=0, \dots, 2^j-1}$.

Let $\{a_{j,k}\}_{j=0,1, \dots, k=0, \dots, 2^j-1}$ be the wavelet coefficients of f , from Lemma 1 below, $a_{j,k} \geq 0$ for all j, k .

[2] Apply the threshold:

$$\hat{a}_{j,k} = \begin{cases} 0 & \text{if } y_{j,k} \leq \lambda_j \\ y_{j,k} - \lambda_j & \text{if } y_{j,k} > \lambda_j \end{cases} \quad (2)$$

to the empirical wavelet coefficients $\{y_{j,k}\}$, with some optimally chosen threshlod λ_j , usually $\lambda_j = \sigma \sqrt{2 \log(n)/n}$ for all levels.

[3] Invert the Haar tranform to get an estimate \hat{f}_i of f_i .

We will discuss some theoretical properties of the estimator in section 2. In section 3, we will compare our estimator with the Grenander estimate both theoretically and numerically.

2 Theoretical Results

The Haar basis is an orthonormal basis of $L_2[0, 1]$ and it is also an interpolating wavelet basis (Donoho, 1992), therefore the wavelet coefficients for the sampled version is essentially the same as those of function version.

We first mention some results on the function version coefficients. Let

$$\phi(t) = I_{[0,1)}(t), \quad \psi(t) = I_{[0,1/2)}(t) - I_{[1/2,1)}(t)$$

and define

$$\psi_{j,k}(t) = 2^{j/2} \psi(2^j t - k)$$

For $f \in L_2[0, 1]$, define the wavelet coefficients

$$b_0 = \int f \phi, \quad a_{j,k} = \int f \psi_{j,k} \quad (3)$$

and for $0 \leq t \leq 1$,

$$f(t) = b_0 + \sum_{j \geq 0} \sum_{k=0}^{2^j-1} a_{j,k} \psi_{j,k}(t)$$

(in the sense of L_2). Moreover, there is the extremely useful Parseval relation:

$$\|\hat{f} - f\|_{L_2[0,1]}^2 = (\hat{b}_0 - b_0)^2 + \sum_{j,k} (\hat{a}_{j,k} - a_{j,k})^2$$

Consider the class of decreasing functions on $[0, 1]$:

$$\mathcal{D}(C) = \{f : f \text{ decreasing and } f(0) - f(1) \leq C\}$$

Lemma 1 Suppose $f \in \mathcal{D}(C)$ and $a_{j,k}$'s are defined as in (3), then

$$a_{j,k} \geq 0$$

for all $j \geq 0$ and $0 \leq k < 2^j$. And furthermore,

$$2^{j/2} \sum_{k=0}^{2^j-1} a_{j,k} \leq C/2$$

for all $j \geq 0$.

Proof: For $j \geq 0$ and $k = 0, 1, \dots, 2^j - 1$,

$$\begin{aligned}
 a_{j,k} &= \int_0^1 f(x)\psi_{j,k}(x)dx = 2^{-j/2} \int_0^1 f\left(\frac{y+k}{2^j}\right)\psi(y)dy \\
 &= 2^{-(j+2)/2} \int_0^1 \left\{f\left(\frac{y+2k}{2^{j+1}}\right) - f\left(\frac{y+2k+1}{2^{j+1}}\right)\right\}dy \\
 &\leq 2^{-j/2} \left(f\left(\frac{k}{2^j}\right) - f\left(\frac{k+1}{2^j}\right)\right) \frac{1}{2}
 \end{aligned} \tag{4}$$

The non-negativity of $a_{j,k}$ is obvious from (4) and

$$2^{j/2} \sum_{k=0}^{2^j-1} a_{j,k} \leq \frac{1}{2} \sum_{k=0}^{2^j-1} \left(f\left(\frac{k}{2^j}\right) - f\left(\frac{k+1}{2^j}\right)\right) = \frac{f(0) - f(1)}{2} \leq C/2$$

This completes the proof.

Next Lemma gives the optimal rate under L_2 norm:

Lemma 2 (Minimax L_2 Risk)

$$\inf_{\hat{f}} \sup_{f \in \mathcal{D}(C)} R(\hat{f}, f) \asymp n^{-2/3}$$

Let

$$\hat{f}_w(t) = \hat{b}_0 + \sum_{j=0}^{m-1} \sum_{k=0}^{2^j-1} \hat{a}_{j,k} \psi_{j,k}(t)$$

be the wavelet estimate of f , as we described earlier, the following Theorem says that \hat{f}_w enjoys the optimal (or near optimal) rate of convergence.

Theorem 1

$$\inf_{\{\lambda_j\}} \sup_{f \in \mathcal{D}(C)} R(\hat{f}_w, f) \asymp n^{-2/3}$$

For $\lambda_j \equiv \sigma \sqrt{2 \log(n)/n}$,

$$\sup_{f \in \mathcal{D}(C)} R(\hat{f}_w, f) \leq C \left(\frac{\log n}{n}\right)^{2/3} (1 + o(1))$$

The proof is in the Appendix.

Remark: In practice, σ^2 , the noise level of the data, is usually unknown. It is natural to find an estimator $\hat{\sigma}$, say, to replace the unknown σ in the thresholds. In this paper, $\hat{\sigma}$ is derived from a linear estimate of f

$$\hat{\sigma}^2 = \sum_{j=[m/2]}^{m-1} \sum_{k=0}^{2^j-1} y_{j,k}^2 \quad (5)$$

Since $y_{j,k}$ are independently $N(a_{j,k}, \sigma^2/n)$ distributed,

$$\frac{n\hat{\sigma}^2}{\sigma^2} \sim \chi_{n-\sqrt{n}}^2(\delta_n)$$

is non-central χ^2 distributed with the non-centrality

$$\delta_n^2 = \sum_{j=[m/2]}^{m-1} \sum_{k=0}^{2^j-1} \frac{na_{j,k}^2}{\sigma^2}$$

and for $f \in \mathcal{D}(C)$, from Lemma 1 and Jensen's inequality,

$$\delta_n^2 \leq \frac{n}{\sigma^2} \left(\sum_{j=[m/2]}^{m-1} \sum_{k=0}^{2^j-1} |a_{j,k}| \right)^2 \leq \frac{n}{\sigma^2} \left(\sum_{j=[m/2]}^{\infty} \frac{C}{2^{j/2}} \right)^2 = \frac{2C^2\sqrt{n}}{\sigma^2(\sqrt{2}-1)^2}$$

By calculating the first and second moments of the non-central χ^2 distribution, for $X \sim \chi_n^2(\delta)$, $EX = n + \delta^2$ and $Var(X) = 2n + 4\delta^2$, we have

$$E(\hat{\sigma}^2 - \sigma^2)^2 = O(n^{-1})$$

Finally, by using the inequality

$$(\sqrt{x} - \sqrt{y})^2 \leq \frac{(x-y)^2}{y}$$

for all $x \geq 0$ and (fixed) $y > 0$, we have

$$E(\hat{\sigma} - \sigma)^2 = O(n^{-1})$$

and this leads to:

Theorem 2 For $\lambda_j \equiv \hat{\sigma}\sqrt{2\log(n)/n}$,

$$\sup_{f \in \mathcal{D}(C)} R(\hat{f}_w, f) \leq C' \left(\frac{\log n}{n} \right)^{2/3} (1 + o(1))$$

The proof is also in the Appendix.

3 Comparisons with LS Estimator

Least square method are commonly used in regression analysis. The LS estimate for f is

$$\hat{f} = \arg \min_{f_1 \geq \dots \geq f_n} \sum_{i=1}^n (y_i - f_i)^2 \quad (6)$$

Note that $\{\hat{f}_i\}$ are also the maximum likelihood estimates of $\{f_i\}$ when $\{z_i\}$ are iid Gaussian random variables.

An effective algorithm, Pool-Adjacent-Violators Algorithm, has been described in §1.2 of Barlow *et al* (1972) and the resulting estimator is usually called the least concave majorant estimator or Grenander estimator, ref. Grenander (1956), Prakasa Rao (1983). Properties of Grenander estimator can also be found in Bergé (1989) and Wang (1991). For example:

Lemma 3 *Let \hat{f}_G be the Grenander estimator, then*

$$\sup_{f \in \mathcal{D}(C)} R(\hat{f}_G, f) \asymp n^{-2/3}$$

i.e. *Grenander estimator achieves the optimal rate.*

We have the following comparison:

- Wavelet estimate equipped with the optimal threshold achieves the optimal rate as the Grenander estimate does; while the estimator with the simple shrinkage rule of using $\lambda_j \equiv \hat{\sigma} \sqrt{2 \log(n)/n}$ is within a factor $(\log n)^{2/3}$ of the optimal rate.
- Computationally, wavelet procedure is more efficient than Grenander procedure. In fact, the computational effort of the wavelet procedure is of order $n \log n$ comparing with order n^2 of the Grenander procedure.
- Grenander estimator has boundary effects. In fact, it does not converge at discontinuous points, Wang (1991). This drawback can be seen from our simulations, while the wavelet estimates do not have boundary effects.

As a final remark, we should mention here is that wavelet procedure does not guarantee us a decreasing solution. From Lemma 1, non-negativity of the Haar coefficients is only a necessary condition for f to be decreasing.

In the case where a decreasing solution is needed, we can still use wavelet procedure as the first step, since wavelet procedure is a rate-preserve transformation. We can then apply Grenander procedure to the transformed data. This two-step procedure requires less computational effort than applying Grenander procedure to the original data.

Numerical examples (Figure 1, 2, 3) show that the wavelet estimate is also competitive numerically with the Grenander estimate. In our simulations, we compare the L_1 and L_2 losses of both Grenander estimator and our wavelet estimator:

$$\begin{aligned} R1 &= \sum_{i=1}^n |\hat{f}(t_i) - f(t_i)| \\ R2 &= \sum_{i=1}^n (\hat{f}(t_i) - f(t_i))^2 \end{aligned}$$

4 Appendix

To prove our main theorem, we need to introduce some basic facts of Besov space theory. Let's define Besov Body in sequence space l_p

$$\Theta_{p,q}^s(C) = \{\theta = (\theta_{j,k})_{j \geq 0, 0 \leq k < 2^j} : \sum_{j=0}^{\infty} \{2^{jsq} (\sum_{k=0}^{2^j-1} |\theta_{j,k}|^p)^{q/p}\} \leq C\}$$

for $q < \infty$ and

$$\Theta_{p,\infty}^s(C) = \{\theta = (\theta_{j,k})_{j \geq 0, 0 \leq k < 2^j} : \sup_{j \geq 0} \{2^{jsp} \sum_{k=0}^{2^j-1} |\theta_{j,k}|^p\} \leq C^p\}$$

Proof of Theorem 1: From Lemma 1, it is obvious that

$$\Theta_D(C) \subset \Theta_+ \cap \Theta_{1,\infty}^{1/2}(C/2) \quad (7)$$

where $\Theta_+ = \{(\theta_{j,k}) : \theta_{j,k} \geq 0\}$.

Therefore,

$$\begin{aligned} \sup_{f \in \mathcal{D}(C)} E\|\hat{f}_w - f\|_{L_2[0,1]}^2 &= \sup_{a \in \Theta_D(C)} E\|\hat{a} - a\|_{l_2}^2 \\ &\leq \sup_{a \in \Theta_+ \cap \Theta_{1,\infty}^{1/2}(C/2)} E\|\hat{a} - a\|_{l_2}^2 \end{aligned}$$

It is well known that (Donoho and Johnstone, 1992a, b)

$$\inf_{\tilde{a}} \sup_{a \in \Theta_{1,\infty}^{1/2}(C/2)} E\|\tilde{a} - a\|_{l_2}^2 \asymp n^{-2/3}$$

and for the shrinkage estimates \hat{a} equipped with the optimal thresholds, we have the same rate

$$\sup_{a \in \Theta_{1,\infty}^{1/2}(C/2)} E\|\hat{a} - a\|_{l_2}^2 \asymp n^{-2/3}$$

for the shrinkage estimate \hat{a} equipped with thresholds $\lambda_j = \sigma\sqrt{2\log(n)/n}$,

$$\sup_{a \in \Theta_{1,\infty}^{1/2}(C/2)} E\|\hat{a} - a\|_{l_2}^2 \leq C'(\frac{\log n}{n})^{2/3}$$

Let \hat{a}_+ be the projection of \hat{a} onto $\Theta_+ \cap \Theta_{1,\infty}^{1/2}(C/2)$, then we have

$$\sup_{a \in \Theta_+ \cap \Theta_{1,\infty}^{1/2}(C/2)} E\|\hat{a}_+ - a\|_{l_2}^2 \asymp n^{-2/3}$$

when the optimal thresholds are used, and

$$\sup_{a \in \Theta_+ \cap \Theta_{1,\infty}^{1/2}(C/2)} E\|\hat{a}_+ - a\|_{l_2}^2 \leq C'(\frac{\log n}{n})^{2/3}$$

when thresholds $\lambda_j = \sigma\sqrt{2\log(n)/n}$ are used.

It is obvious that the coordinates in \hat{a}_+ have the expressions in (2).

Proof of Theorem 2: The proof follows immediately from Theorem 1 and the following Lemma.

Lemma 4

$$\sum_{j=0}^{m-1} \sum_{k=0}^{2^j-1} |E(\hat{a}_{j,k} - a_{j,k})^2 - E(\hat{a}_{j,k} - a_{j,k})^2| = o(n^{-2/3})$$

Proof: From the definitions of $\hat{a}_{j,k}$ and $\hat{a}_{j,k}$,

$$\begin{aligned} & |(\hat{a}_{j,k} - a_{j,k})^2 - (\hat{a}_{j,k} - a_{j,k})^2| \\ & \leq \frac{\lambda^2}{n} (\hat{\sigma} - \sigma)^2 + \frac{2\lambda\sigma}{n} |z_{j,k}| |\hat{\sigma} - \sigma| I_{[z_{j,k} > \lambda(\frac{\hat{\sigma} \wedge \sigma}{\sigma} - \frac{\sqrt{n}a_{j,k}}{\sigma\lambda})]} \end{aligned}$$

where $z_{j,k} = \sqrt{n}(w_{j,k} - a_{j,k})/\sigma$. So

$$\begin{aligned} & |E(\hat{a}_{j,k} - a_{j,k})^2 - E(\hat{a}_{j,k} - a_{j,k})^2| \\ & \leq \frac{\lambda^2}{n} E(\hat{\sigma} - \sigma)^2 + \frac{2\lambda\sigma}{n} E\{|z_{j,k}| |\hat{\sigma} - \sigma| I_{[z_{j,k} > \lambda(\frac{\hat{\sigma} \wedge \sigma}{\sigma} - \frac{\sqrt{n}a_{j,k}}{\sigma\lambda})]}\} \\ & \leq \frac{\lambda^2}{n} E(\hat{\sigma} - \sigma)^2 + \frac{2\lambda\sigma}{n} (E|z|^{1/\beta})^\beta \sqrt{E(\hat{\sigma} - \sigma)^2} P\{z > \lambda(\frac{\hat{\sigma}}{\sigma} \wedge 1 - \frac{\sqrt{n}a_{j,k}}{\sigma\lambda})\}^{\frac{1}{2}-\beta} \\ & \leq O(\frac{\log n}{n^2}) + O(\frac{\sqrt{\log n}}{n^{3/2}}) P\{z > \lambda(\frac{\hat{\sigma}}{\sigma} \wedge 1 - \frac{\sqrt{n}a_{j,k}}{\sigma\lambda})\}^{\frac{1}{2}-\beta} \end{aligned}$$

where $z \sim N(0, 1)$, $0 < \beta < 1/2$.

For those $a_{j,k}$ satisfying

$$\frac{\sqrt{n}a_{j,k}}{\sigma\lambda} \leq r$$

where $0 < r < 1$. Let Z_n be a standardized non-central $\chi^2_{n-\sqrt{n}}(\delta_n)$ variate (i.e. $EZ_n = 0$ and $Var(Z_n) = 1$) and $s \in (r, 1)$,

$$\begin{aligned} & P\{z > \lambda(\frac{\hat{\sigma}}{\sigma} \wedge 1 - \frac{\sqrt{n}a_{j,k}}{\sigma\lambda})\} \\ & \leq P\{z > \lambda(\frac{\hat{\sigma}}{\sigma} \wedge 1 - r)\} \\ & \leq P\{z > \lambda(\frac{\hat{\sigma}}{\sigma} \wedge 1 - r), \hat{\sigma} \geq s\sigma\} + P\{\hat{\sigma} < s\sigma\} \\ & \leq P\{z > \lambda(s - r)\} + P\{\chi^2_{n-\sqrt{n}}(\delta_n) < s^2 n\} \\ & \leq \frac{\phi(\lambda(s - r))}{\lambda(s - r)} + P\{|Z_n| > \frac{(1 - s^2)n + \delta_n^2}{\sqrt{2n + 4\delta_n^2}}\} \end{aligned}$$

$$\begin{aligned}
&= O\left(\frac{1}{n^{(s-r)^2}\sqrt{\log n}}\right) + O(n^{-1}) \\
&= O\left(\frac{1}{n^{(s-r)^2}\sqrt{\log n}}\right)
\end{aligned}$$

Consider

$$N_n = \#\left\{\frac{\sqrt{n}a_{j,k}}{\sigma\lambda} > r, 0 \leq j < m, 0 \leq k < 2^j\right\}$$

where $m = \log_2 n$. Then for $f \in \mathcal{D}(C)$, from Lemma 1,

$$\frac{\sqrt{2}C}{\sqrt{2}-1} \geq \sum_{j=0}^{m-1} \frac{C}{2^{j/2}} \geq \sum_{j=0}^{m-1} \sum_{k=0}^{2^j-1} a_{j,k} \geq \sum_{a_{j,k} > r\sigma\lambda/\sqrt{n}} a_{j,k} \geq \frac{r\sigma\lambda N_n}{\sqrt{n}}$$

and so

$$N_n \leq \frac{\sqrt{2n}C}{(\sqrt{2}-1)r\sigma\lambda} \quad (8)$$

Therefore, by choosing r, β small and s close to 1 such that

$$(s-r)^2(1/2-\beta) > 1/6$$

we have

$$\begin{aligned}
&\sum_{j=0}^{m-1} \sum_{k=0}^{2^j-1} |E(\hat{a}_{j,k} - a_{j,k})^2 - E(\hat{a}_{j,k} - a_{j,k})^2| \\
&= \sum_{j=0}^{m-1} \sum_{k=0}^{2^j-1} \left\{ O\left(\frac{\log n}{n^2}\right) + O\left(\frac{\sqrt{\log n}}{n^{3/2}}\right) P\left\{ z > \lambda\left(\frac{\hat{\sigma}}{\sigma} \wedge 1 - \frac{\sqrt{n}a_{j,k}}{\sigma\lambda}\right)^{\frac{1}{2}-\beta}\right\} \right\} \\
&= O\left(\frac{\log n}{n}\right) + O\left(\frac{\sqrt{\log n}}{n^{3/2}}\right) \sum_{j=0}^{m-1} \sum_{k=0}^{2^j-1} P\left\{ z > \lambda\left(\frac{\hat{\sigma}}{\sigma} \wedge 1 - \frac{\sqrt{n}a_{j,k}}{\sigma\lambda}\right)^{\frac{1}{2}-\beta}\right\} \\
&= O\left(\frac{\log n}{n}\right) + O\left(\frac{\sqrt{\log n}}{n^{3/2}}\right) \left\{ \sum_{a_{j,k} \leq r\sigma\lambda/\sqrt{n}} \frac{1}{n^{(s-r)^2(1/2-\beta)}\sqrt{\log n}} + \sum_{a_{j,k} > r\sigma\lambda/\sqrt{n}} 1 \right\} \\
&= O\left(\frac{\log n}{n}\right) + O\left(\frac{\sqrt{\log n}}{n^{3/2}}\right) \left(\frac{n}{n^{(s-r)^2(1/2-\beta)}\sqrt{\log n}} + \sqrt{\frac{n}{\log n}} \right) \\
&= o(n^{-2/3})
\end{aligned}$$

This completes the proof of the Lemma.

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Figure 1

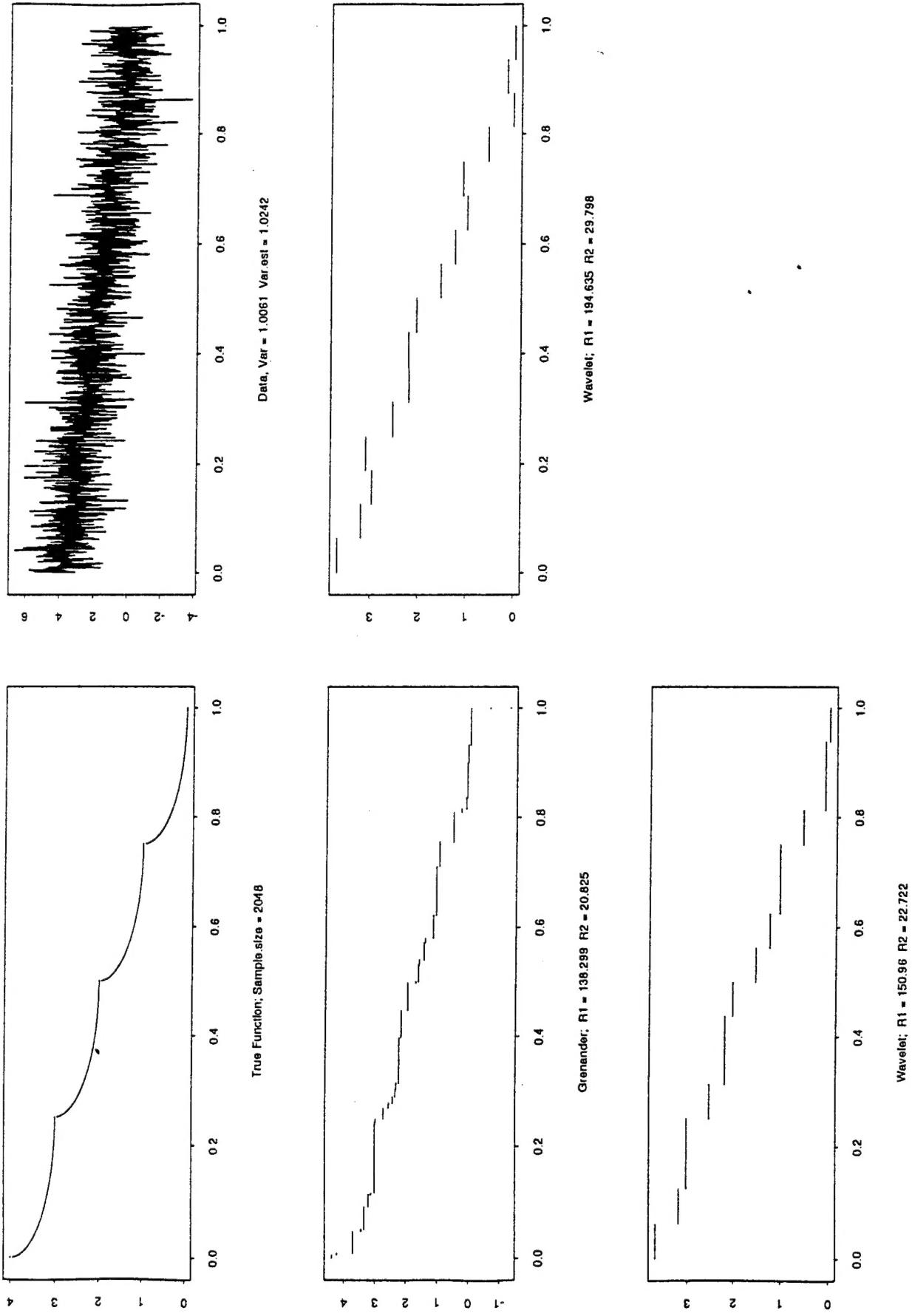


Figure 2

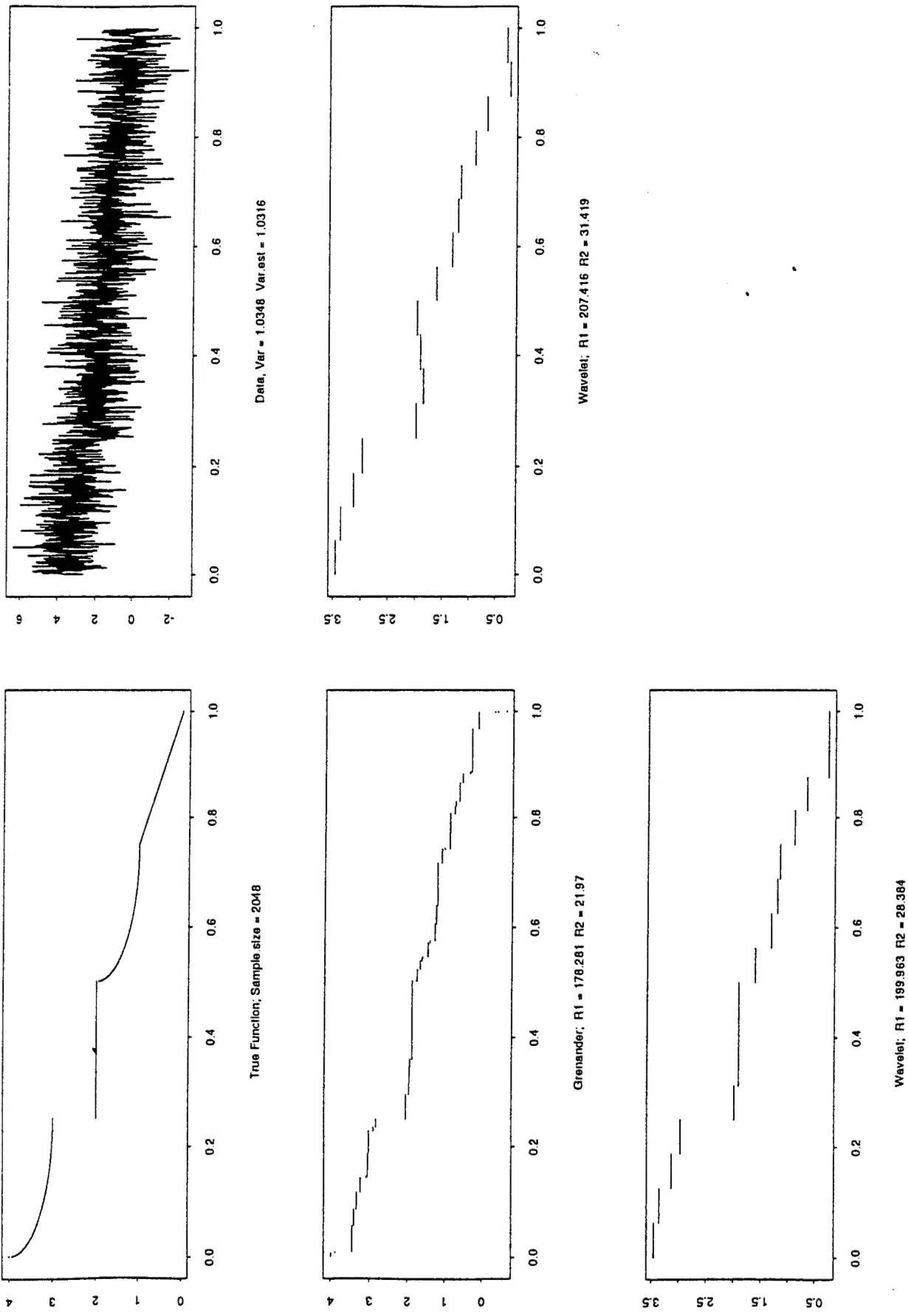


Figure 3

